Approaching condensed matter ground states from below

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We present a generic approach to the condensed matter ground state problem which is complementary to variational techniques and works directly in the thermodynamic limit. Relaxing the ground state problem, we obtain semidefinite programs (SDP). These can be solved efficiently, yielding lower bounds to the ground state energy and approximations to the few-particle Green's functions. As the method is applicable for all particle statistics, it represents in particular a novel route for the study of strongly correlated fermionic and frustrated spin systems in $D > 1$ spatial dimensions. It is demonstrated for the XXZ model and the Hubbard model of spinless fermions. The results are compared against exact solutions, Quantum Monte Carlo, and Anderson bounds, showing the competitiveness of the SDP method.

I. INTRODUCTION

Prominent simulation techniques for condensed matter systems are sampling algorithms like *Quantum Monte Carlo* (QMC) [1–4] and variational algorithms like the *density-matrix renormalization-group* (DMRG) [5, 6], other *tensor network state* (TNS) approaches [7–10], or *variational Monte Carlo* (VMC) [11–14]. For a number of interesting classes of systems, like frustrated or fermionic systems in $D > 1$ spatial dimensions, the powerful QMC technique is hampered by the *sign problem* [15–17]. Hence, such systems are then often studied with variational techniques, minimizing the energy within a certain class of states as, e.g., TNS of a certain structure. The energy expectation value of the obtained state is necessarily an upper bound to the exact ground state energy.

In this article, a complementary approach is presented. By relaxations of the ground state problem, one obtains *semidefinite programs* (SDP) [18, 19], which can be solved efficiently on classical computers and yield lower bounds to the ground state energy and corresponding approximations to few-particle Green's functions. The obtained Green's functions allow, e.g., for the study of phase diagrams. As the presented SDP method works irrespective of the particle statistics, it provides in particular a novel route for the study of strongly correlated fermionic and frustrated spin systems for $D > 1$. The method can also be used to judge the quality of variational algorithms in situations where exact or QMC results are not available for comparison. This is especially important for VMC methods [13, 14] and the recently developed variational TNS techniques for fermions in $D > 1$ [20–24].

The idea is to specify the system by its k-point Green's functions $\mathcal{G}^{(k)}$. For systems of fermions, bosons, or hard-core bosons (being equivalent to spins-1/2) in a normalized state $\hat{\rho}$, they read

$$\mathcal{G}^{(k)}_{\boldsymbol{i},\boldsymbol{j}} := \mathrm{Tr}(\hat{\rho}\,\hat{a}_{i_m}\dots\hat{a}_{i_1}\hat{a}^\dagger_{j_1}\dots\hat{a}^\dagger_{j_n}), \quad k = m+n, \qquad (1)$$

where $\{\hat{a}_i, \hat{a}_i^\dagger\}_i$ denote the ladder operators with respect to some single-particle basis states $|i\rangle$; [25]. The energy expectation value $E = \mathrm{Tr}\,\hat{\rho}\hat{H}$ is a function of the (few-particle) Green's functions, i.e., $E = E(\mathcal{G})$. The exact ground state energy would be obtained by minimizing it among all *representable* Green's functions $\mathcal{G}$, i.e., those for which a density operator $\hat{\rho}$ exists, such that Eq. (1) is obeyed. To determine whether a given Green's function G is representable turns out to be a computationally hard problem, the famous *N-representability problem* [26–29], which is QMA-complete [30]. An efficient minimization of E is however possible if we relax the constraints on the Green's function, then, yielding not the exact ground state energy but a lower bound, and not the exact ground state Green's function but an approximation. Note that minimizing $E(G)$ without any constraints is doomed to fail as the energy is linear in G. Manageable constraints on G can be constructed by imposing the positivity of the expectation values of certain positive-definite observables like, e.g., the particle density operator $\hat{a}_i^\dagger\hat{a}_i$, and so on. Such an approach for fermionic $G^{(1)}$ and $G^{(2)}$ has been successfully applied in quantum chemistry; see, e.g., [31] and references therein.

Here, we present a systematic method for the construction and solution of relaxed ground state problems for condensed matter systems. Similar to the approach known from quantum chemistry, our constraints enforce positive expectation values for operators of the form $\hat{C}^\dagger\hat{C}$ with respect to the Green's functions G. More generally than before, we (a) choose the *constraint operators* $\hat{C}$ to be arbitrary polynomials of degree $\leq K$ in the ladder operators, which (b) act on suitably chosen subsets of the lattice. We (c) exploit the translation invariance of the condensed matter systems to (d) work effectively with an infinite number of degrees of freedom and describe the systems directly in the thermodynamic limit. The method yields coupled constraints for $G^{(1)},\dots,G^{(2K)}$ such that the energy optimization problem attains the form of an SDP. On basis of the bipolar theorem [32], we further elucidate the mathematical background of the method and further possible reductions to the number of constraints.

An alternative method for calculating lower bounds to

the ground state energy is due to Anderson. *Anderson bounds* [33, 34] are obtained by splitting the Hamiltonian $\hat{H}$ into a sum of subsystem Hamiltonians $\hat{H}_m$ that are accessible by exact diagonalization. The Anderson bound for the ground state energy E^0 is then given by the sum of the ground state energies E^0_m of the $\hat{H}_m$,

$$\hat{H} = \sum_m \hat{H}_m \quad \Rightarrow \quad E^0 \geq \sum_m E^0_m. \tag{2}$$

The computation cost for this bound scales exponentially in the spatial supports of the operators $\hat{H}_m$; see Appx. B.

In contrast, the computation cost for the SDP method scales only polynomially in the support of the constraint operators. In the prominent systems that we studied with moderate computer resources, the SDP method typically outperforms the Anderson bound. The SDP method has the additional advantage of giving access to translation-invariant Green's functions, which can be used to study phase diagrams etc.. Furthermore, it is possible to choose different spatial supports of the constraint operators $\hat{C}$ depending on their degree in the ladder operators. The optimal choice for those spatial supports depends on the position in the phase diagram.

II. GROUNDSTATE PROBLEM

The following description applies to lattice systems of fermions, bosons, and hardcore bosons – each corresponding to a certain algebra for the ladder operators $\{a_i\}_i$ [25]. Spins-1/2 can be treated by mapping them to hardcore bosons via the identification $\hat{a}_i = \hat{S}^-_i$, $\hat{a}^\dagger_i = \hat{S}^+_i$, and $\hat{S}^z_i = \hat{a}^\dagger_i \hat{a}_i - \frac{1}{2}$. The generalization to higher spins is straightforward. For each subset Ω of the single-particle modes $\{|i\rangle\}$, let $\mathcal{A}^k_\Omega$ denote the operator basis of normal-ordered monomials of degree k in the ladder operators for subsystem Ω.

$$\mathcal{A}^k_\Omega := \{\hat{a}_{i_m} \dots \hat{a}_{i_1} \hat{a}^\dagger_{i_{m+1}} \dots \hat{a}^\dagger_{i_k} \,|\, 0 \leq m \leq k,\, i_\ell \in \Omega\} \tag{3}$$

Each density operator $\hat{\rho}$ corresponds to a representable Green's function $\mathcal{G}$, with its k-point component given by

$$\mathcal{G}^{(k)}_{\hat{\sigma}} := \operatorname{Tr} \hat{\rho}\hat{\sigma} \quad \text{for} \quad \hat{\sigma} \in \mathcal{A}^k_\Omega. \tag{4}$$

For the moment, let us choose Ω to be the full system. Every linear operator $\hat{B}$ on the Hilbert space can be expanded in the basis $\mathcal{A} := \bigcup_k \mathcal{A}^k$ as $\hat{B} = \sum_{\hat{\sigma}\in\mathcal{A}} B_{\hat{\sigma}} \hat{\sigma}$. Its expectation value with respect to a state $\hat{\rho}$ is then

$$\operatorname{Tr} \hat{\rho}\hat{B} = \sum_{\hat{\sigma}\in\mathcal{A}} \mathcal{G}_{\hat{\sigma}} B_{\hat{\sigma}} =: \mathcal{G}[\hat{B}], \tag{5}$$

where $\mathcal{G}$ is the Green's function of $\hat{\rho}$. In this sense, Green's functions are linear functionals on the operators.

For a Hamiltonian $\hat{H}$, the ground state problem reads

$$E^0 = \min_{\hat{\rho}\in\mathcal{D}} \operatorname{Tr} \hat{\rho}\hat{H} = \min_{\mathcal{G}\in\mathcal{R}} \mathcal{G}[\hat{H}], \tag{6}$$

where $\mathcal{D}$ denotes the set of all density operators and $\mathcal{R}$ denotes the set of all representable Green's functions,

$$\begin{aligned}\mathcal{R} :&= \{\mathcal{G} \,|\, \exists\, \hat{\rho} \in \mathcal{D} :\, \mathcal{G}_{\hat{\sigma}} = \operatorname{Tr} \hat{\rho}\hat{\sigma} \;\; \forall_{\hat{\sigma}\in\mathcal{A}}\} \\ &= \{\mathcal{G} \,|\, \mathcal{G}[\mathrm{Id}] = 1,\, \mathcal{G}_{\hat{\sigma}^\dagger} = \mathcal{G}^*_{\hat{\sigma}},\, \mathcal{G}[\hat{B}] \geq 0 \;\; \forall_{\hat{B}\succeq 0}\}. \end{aligned} \tag{7}$$

This equality follows from the fact that the only constraints on a valid density operator $\hat{\rho}$ are $\operatorname{Tr} \hat{\rho} = 1$, $\hat{\rho} = \hat{\rho}^\dagger$, and its positivity $\hat{\rho} \succeq 0$ which is equivalent to requiring $\operatorname{Tr} \hat{\rho}\hat{B} \geq 0$ for all positive semidefinite operators $\hat{B} \succeq 0$.

Variational methods proceed from Eq. (6) by choosing some accessible subset of $\mathcal{D}$. Each variational state from such a subset yields an upper bound to the ground state energy E^0. In contrast, for the SDP method, described in the following, one chooses an accessible superset $\mathcal{F}$ of the set $\mathcal{R}$ of representable Green's functions, i.e., relaxes the constraints. Minimizing the energy in such a superset yields a lower bound to E^0. A decisive feature of the SDP method is that the minimum energies for the chosen supersets $\mathcal{F}$ can be found certifiably; see Appx. A.

III. SDP METHOD

Solving the ground state problem (6) in general is known to be a computationally hard problem; it is QMA-complete [35]. Similarly, determining whether given Green's functions are representable, i.e., elements of $\mathcal{R}$ in Eq. (7), is also a QMA-complete problem [30].

A straightforward way to relax the – apparently too demanding – constraints represented by $\mathcal{R}$ is to require the Green's functional $G[\hat{B}]$ to be non-negative not for all $\hat{B} \succeq 0$, but only for operators $\hat{B}$ of the form $\hat{B} = \hat{C}^\dagger \hat{C}$ with constraint operators $\hat{C}$ from some set $\mathcal{C}$. Minimizing the energy $G[\hat{H}]$ with respect to Green's functions G from the set

$$\mathcal{F}_\mathcal{C} := \{G \,|\, G[\mathrm{Id}] = 1,\, G_{\hat{\sigma}^\dagger} = G^*_{\hat{\sigma}},\, G[\hat{C}^\dagger \hat{C}] \geq 0 \;\; \forall_{\hat{C}\in\mathcal{C}}\}, \tag{8}$$

yields a lower bound to the ground state energy (6).

$$E^0 \geq \min_{G\in\mathcal{F}_\mathcal{C}} G[\hat{H}] \equiv \min_{G\in\mathcal{F}_\mathcal{C}} \sum_{\hat{\sigma}} G_{\hat{\sigma}} H_{\hat{\sigma}}, \tag{9}$$

as $\mathcal{R} \subset \mathcal{F}_\mathcal{C}$. Imposing more and more constraints by enlarging the operator set $\mathcal{C}$, the bound approaches E^0, and the optimal G approaches the ground state Green's function. Determining the optimum in Eq. (9) is a semidefinite programming problem for the variables $G_{\hat{\sigma}}$, as $G[\hat{H}] \equiv \sum_{\hat{\sigma}} G_{\hat{\sigma}} H_{\hat{\sigma}}$ is linear in G, and the constraints $G[\hat{C}^\dagger \hat{C}] \geq 0 \;\forall \hat{C} \in \mathcal{C}$ can be written in the form

$$\sum_{\hat{\sigma}} G_{\hat{\sigma}} M_{\hat{\sigma}} \succeq 0, \tag{10}$$

where the Hermitian matrices $M_{\hat{\sigma}}$ are completely determined by the underlying algebra of the ladder operators $\hat{a}_i$ and the choice for the constraint operator set $\mathcal{C}$. Eqs. (9) and (10) correspond to a standard form

for an SDP [18, 19]; see also Appx. A. Eq. (10) results from expanding the constraint operators in the basis $\mathcal{A}$, $\hat{C} = \sum_{\hat{\sigma}} C_{\hat{\sigma}} \hat{\sigma}$. This yields the constraints in the form $\sum_{\hat{\sigma}'\hat{\sigma}''} C^*_{\hat{\sigma}'} G[(\hat{\sigma}')^\dagger \hat{\sigma}''] C_{\hat{\sigma}''} \geq 0 \ \forall_{\boldsymbol{C}}$. Expanding the operators $(\hat{\sigma}')^\dagger \hat{\sigma}''$ in the operator basis $\mathcal{A}$ (by bringing them into normal-ordered form) and using $G[\hat{\sigma}] \equiv G_{\hat{\sigma}}$ yields the matrices $[M_{\hat{\sigma}}]_{\hat{\sigma}',\hat{\sigma}''}$ and the constraints

$$\sum_{\hat{\sigma}\hat{\sigma}'\hat{\sigma}''} G_{\hat{\sigma}} C^*_{\hat{\sigma}'} [M_{\hat{\sigma}}]_{\hat{\sigma}',\hat{\sigma}''} C_{\hat{\sigma}''} = \sum_{\hat{\sigma}} G_{\hat{\sigma}} \boldsymbol{C}^\dagger M_{\hat{\sigma}} \boldsymbol{C} \geq 0 \quad \forall_{\boldsymbol{C}}$$

from which Eq. (10) follows.

IV. THERMODYNAMIC LIMIT AND CONSTRAINT OPERATORS

Let us now turn to the specific case of condensed matter systems in the thermodynamic limit. Let the Hamiltonian be translation-invariant $\hat{H} = \sum_{\boldsymbol{r}} \mathcal{T}_{\boldsymbol{r}}(\hat{h})$ with finite-range interaction terms $\hat{h}$ and the lattice translation operator $\mathcal{T}_{\boldsymbol{r}}$. We denote the spatial support of the κ-point terms in $\hat{h}$ by Λ_κ. For a particle-number conserving D-dimensional model with 2-body nearest neighbor interactions, this means for example $|\Lambda_2| = |\Lambda_4| = D+1$, and $\Lambda_\kappa = \emptyset \ \forall_{\kappa \neq 2,4}$. Due to the translation invariance of $\hat{H}$, we can restrict ourselves to translation-invariant density matrices and Green's functions. A constraint operator set can be constructed by choosing, for each operator order k, a subsystem Ω_k of the full lattice such that

$$\Omega_{k'} \subseteq \Omega_k \quad \forall_{k,k'>k} \quad \text{and} \quad \Lambda_\kappa \subseteq \Omega_{\lceil \kappa/2 \rceil} \quad \forall_\kappa. \tag{11}$$

Every such choice of subsystems and the corresponding set of constraint operators

$$\mathcal{C}_{\boldsymbol{\Omega}} := \operatorname{span} \mathcal{A}_{\boldsymbol{\Omega}} \quad \text{with} \quad \mathcal{A}_{\boldsymbol{\Omega}} := \bigcup_k \mathcal{A}^k_{\Omega_k} \tag{12}$$

defines with Eq. (8) a set $\mathcal{F}_{\mathcal{C}_{\boldsymbol{\Omega}}} \supset \mathcal{R}$ of Green's functions. The number of Green's function elements $G_{\hat{\sigma}}$ occurring as degrees of freedom in the SDP is then given by the size $|\mathcal{A}_{\boldsymbol{\Omega}}|$ of the operator basis. It depends on the particle statistics: For a given subsystem Ω of a bosonic system, $|\mathcal{A}^k_\Omega|$ grows exponentially in the operator order k. For fermions, hardcore bosons, and spins-1/2, $|\mathcal{A}^k_\Omega|$ initially grows exponentially but drops to zero for $k > 2|\Omega|$. We always choose some K so that $\Omega_k = \emptyset \ \forall_{k>K}$. Enlarging the subsystems Ω_k, systematically improves the solution of Eq. (9) and increases the computation cost polynomially. For given model and computer resources, the optimal choice for the subsystems Ω_k depends on the position in the phase diagram.

V. SYMMETRIES

Hamiltonian symmetries, like translation or rotation invariance, imply that several Green's function elements $G_{\hat{\sigma}}$ can be chosen to be identical (e.g., $G_{\hat{a}_{\boldsymbol{x}}\hat{a}^\dagger_{\boldsymbol{y}}} \equiv G_{\hat{a}_{\boldsymbol{0}}\hat{a}^\dagger_{\boldsymbol{y}-\boldsymbol{x}}} \ \forall_{\boldsymbol{xy}}$) and it is sufficient to use in the SDP only one representative for each of the corresponding equivalence classes. Further, several Green's function elements can be zero (e.g., $G_{\hat{a}_{\boldsymbol{x}}\hat{a}_{\boldsymbol{y}}} = 0$ for particle-number conserving models). A corresponding block structure in $\sum_{\hat{\sigma}} G_{\hat{\sigma}} M_{\hat{\sigma}}$ can be exploited to further reduce the computation cost.

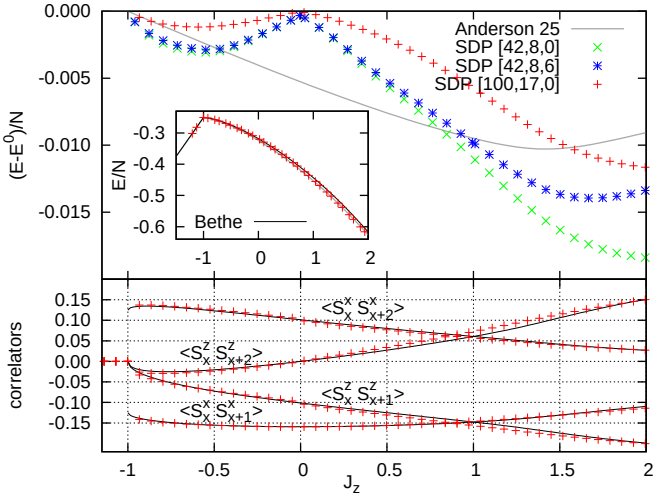

Figure 1: (color online) Lower bounds E to the ground state energy and approximations to correlators for the XXZ chain (13). The Anderson bound (2) was calculated with clusters of 25 sites. The subsystems Ω_k for the SDP method (9) are clusters with sizes $|\Omega_1|$, $|\Omega_2|$, and $|\Omega_3|$ as specified in the legend ($K = 3$). The Bethe ansatz yields the exact ground state energy E^0 and short-range correlators [36, 37].

VI. EXEMPLARY APPLICATIONS

A. XXZ chain

Let us first address the spin-1/2 XXZ model

$$\hat{H} = \sum_{\langle i,j \rangle} (\hat{S}^x_i \hat{S}^x_j + \hat{S}^y_i \hat{S}^y_j + J_z \hat{S}^z_i \hat{S}^z_j) \tag{13}$$

in one spatial dimension (1D). For $J_z < -1$, the model is in a gapped ferromagnetic phase with a fully polarized ground state. In the region $-1 \leq J_z \leq 1$ there is the gapless "XY" phase. For $J_z > 1$, the system is in the gapped antiferromagnetic Néel phase. The phase transition at $J_z = -1$ is of second order and the one at $J_z = 1$ is of Berezinsky-Kosterlitz-Thouless type [38]. Using comparable (moderate) computer resources, the energy bound obtained from the SDP method (9) improves substantially on the Anderson bound (2) in large parts of the phase diagram; Fig. 1. For $J_z = 0$, where the model corresponds to a system of free fermions, the SDP bounds reproduce the exact ground state energy to high precision. Employing higher-order Green's functions tends to improve bounds at larger J_z. The obtained

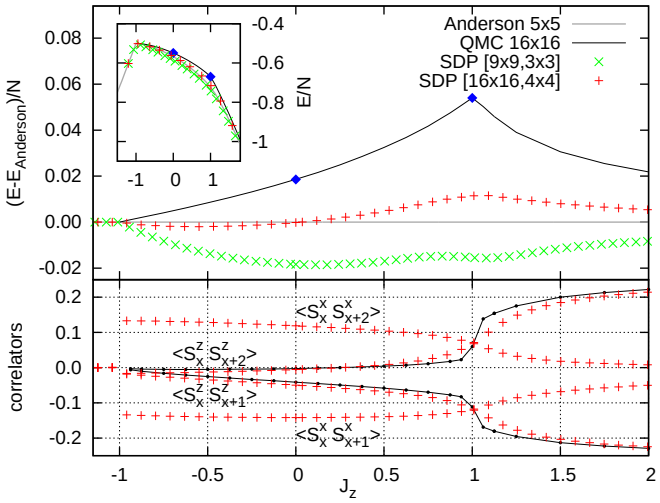

Figure 2: (color online) Lower energy bounds and correlators for the 2D XXZ model, complemented by QMC data calculated for a square lattice of 16×16 sites with periodic boundary conditions, and inverse temperature $\beta = 96$. The QMC energies for $J_z = 0, 1$ coincide with earlier results (⧫) from Ref. [39, 40]. The QMC error bars would be smaller than the line width, and another simulation with a 32x32 lattice produced visually indistinguishable results. We chose SDP constraint subsystems Ω_1 and Ω_2 of square shape with sizes as specified in the legend.

short-range correlators coincide very well with the exact Bethe Ansatz results [36, 37].

B. 2D XXZ model

Let us now consider the spin-1/2 XXZ model (13) on a square lattice. With the identification $\hat{a}_i = \hat{S}_i^-$, $\hat{a}_i^\dagger = \hat{S}_i^+$, $\hat{S}_i^z = \hat{a}_i^\dagger \hat{a}_i - \frac{1}{2}$, it maps to a model of interacting hard-core bosons obeying the algebra $\hat{a}_i \hat{a}_j^\dagger - (-1)^{\delta_{ij}} \hat{a}_i^\dagger \hat{a}_j = \delta_{ij}$. As displayed in Fig. 2, the SDP method can yield better lower bounds to the ground state energy than the Anderson bound. However, with the employed computer resources, the improvement is arguably not as impressive as for the other two studied models. As there is no exact solution available, we also simulated the model with QMC based on the stochastic series expansion [3], showing again that the SDP method gives access to the correlation functions.

C. 2D Hubbard model of spinless fermions

Finally, Fig. 3 shows how the SDP method improves upon Anderson bounds for the 2D Hubbard model of spinless fermions

$$\hat{H} = -\frac{1}{2} \sum_{\langle i,j \rangle} (\hat{a}_i^\dagger \hat{a}_j + h.c.) + U \sum_{\langle i,j \rangle} (\hat{n}_i - \frac{1}{2})(\hat{n}_j - \frac{1}{2}) \quad (14)$$

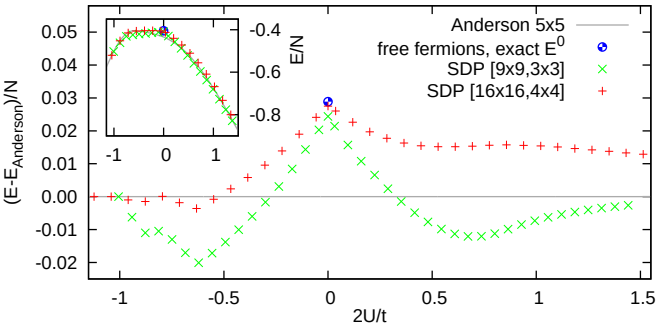

Figure 3: (color online) Lower energy bounds for the 2D Hubbard model of spinless fermions on a square lattice (14).

on a square lattice. In this case, except for $U = 0$, no exact results are available and QMC is inefficient due to the sign problem [15–17].

VII. BIPOLAR THEOREM

Often, one is only interested in the single- and two-particle Green's functions. However, in the presented SDP approach, we also introduce higher Green's functions to improve the approximation. On the basis of the bipolar theorem, one can understand that such higher Green's functions represent slack variables. The set of representable $(k \leq K)$-point Green's functions

$$\tilde{\mathcal{R}}_K := \{\mathcal{G} \,|\, \exists\, \hat{\rho} \in \mathcal{D} : \; \mathcal{G}_{\hat{\sigma}}^{(k)} = \mathrm{Tr}\, \hat{\rho} \hat{\sigma} \;\; \forall_{k \leq K,\, \hat{\sigma} \in \mathcal{A}^k}\}$$

is convex, as $\mathcal{G}$ is linear in $\hat{\rho}$ and $\mathcal{D}$ is convex. Giving up on the (inessential) normalization of the Green's functions, the set $\mathcal{R}_K := \{\alpha \mathcal{G} \,|\, \mathcal{G} \in \tilde{\mathcal{R}}_K,\, \alpha \in \mathbb{R}_+\}$ becomes a convex cone. For a given scalar product, $\langle \cdot, \cdot \rangle$, the bipolar theorem [32] states that $(\mathcal{R}_K^*)^* = \mathcal{R}_K$, where

$$\mathcal{R}_K^* := \{\hat{B} \,|\, \langle B, \mathcal{G} \rangle \geq 0 \;\; \forall_{\mathcal{G} \in \mathcal{R}_K}\} \quad (15)$$

is the polar cone of $\mathcal{R}_K$. With the choice $\langle B, \mathcal{G} \rangle := \sum_k \sum_{\hat{\sigma} \in \mathcal{A}^k} \mathcal{G}_{\hat{\sigma}}^{(k)} B_{\hat{\sigma}} \equiv \mathcal{G}[\hat{B}]$, the polar $\mathcal{R}_K^*$ is the convex cone of all positive semidefinite operators from $\mathcal{B}_K := \mathrm{span} \bigcup_{k=0}^K \mathcal{A}^k$. Due to the bipolar theorem, $\mathcal{R}_K$ is hence characterized by $\mathcal{R}_K^*$ as

$$\mathcal{R}_K = \{\mathcal{G} \,|\, \mathcal{G}_{\hat{\sigma}^\dagger} = \mathcal{G}_{\hat{\sigma}}^* \,\forall_{\hat{\sigma}},\, \mathcal{G}[\hat{B}] \geq 0 \;\; \forall_{\hat{B} \in \mathcal{B}_K,\, \hat{B} \succeq 0}\}. \quad (16)$$

So, to obtain (or approximate) the $(k \leq K)$-point Green's functions, one needs to consider only $(k \leq K)$-point operators $\hat{B} \succeq 0$. In this sense, higher Green's functions are slack variables, which are only employed in order to bring the ground state problem into the form of an SDP; Eqs. (9) and (10). We showed how constraints $G[\hat{B}] \geq 0$ can be enforced in the SDP, for the case that $\hat{B} = \hat{C}^\dagger \hat{C}$ with constraint operators $\hat{C}$ that are polynomials of degree $\leq K/2$. However, there are also subspaces of operators $\hat{C}$ of polynom degree $> K/2$ such that $G[\hat{C}^\dagger \hat{C}]$ can

be evaluated with the $(k \leq K)$-point Green's functions. They can hence be taken into account without introducing higher Green's functions. A particularly simple space of such operators for a particle-number conserving system is given by $\hat{C} = \sum_{\boldsymbol{i}} c_{\boldsymbol{i}} \hat{a}_{i_1} \dots \hat{a}_{i_m} + h.c.$: For every odd m, $G[\hat{C}^\dagger \hat{C}]$ can be evaluated without requiring $G^{(2m)}$.

VIII. CONCLUSION

We have presented a method for calculating lower bounds to the ground state energy of condensed matter systems and approximations to the ground state Green's functions. Based on certain relaxations of the ground state problem one obtains efficiently solvable SDPs. The method can also be used for systems with particles of mixed statistics, higher spins, etc., by employing the corresponding operator algebras. Our generic considerations on the SDP method carry over to quantum chemistry problems. A decisive advantage in the variant for condensed matter systems is, however, that translation invariance and locality can be exploited to systematically balance the number of degrees of freedom and the computation cost.

Acknowledgments

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Appendix A: Semidefinite programming

For the estimation of lower energy bounds we use semidefinite programming (SDP) [18, 19]. The SDP algorithm iteratively approaches the solution of two different but related numerical problems, one corresponding to the lower energy bound we are looking for. Under certain circumstances, the limiting point is a guaranteed optimum of both optimization problems and provides us with a certified lower bound for the energy.

Let Q and M_σ with $\sigma = 1, \dots, m$ be symmetric real matrices and $H \in \mathbb{R}^m$. The first, and so called *primal problem*, is to find

$$p^* := \max_{X \succeq 0} \operatorname{Tr} Q^T X \tag{A1}$$

$$\text{such that } \operatorname{Tr} M_\sigma^T X = H_\sigma \quad \forall\, \sigma. \tag{A2}$$

The second, and so called *dual problem*, is to find

$$d^* := \min_{g \in \mathbb{R}^m} \sum_{\sigma=1}^m g_\sigma H_\sigma \tag{A3}$$

$$\text{such that } \sum_{\sigma=1}^m g_\sigma M_\sigma - Q \succeq 0. \tag{A4}$$

The dual problem is our energy minimization problem if we let $g_\sigma = G_{\hat{\sigma}}$ be the the Green's function, $M_\sigma = M_{\hat{\sigma}}$ the constraint matrices occurring in the positivity condition Eq. (10), and H the Hamiltonian in its vectorized representation. Let also $Q = -M_{\mathrm{Id}}$, without coefficient, because $G_{\mathrm{Id}} \equiv 1$ is fixed, as it corresponds to the norm of the state we are searching for.

We always have that $p^* \leq d^*$, because the cone of positive semidefinite matrices is self-dual, implying $X, Y \succeq 0 \Rightarrow \operatorname{Tr} X^T Y \geq 0$ and, hence,

$$\begin{aligned} 0 &\leq \operatorname{Tr}\big(\sum_{\sigma=1}^m g_\sigma M_\sigma - Q\big)^T X = \sum_{\sigma=1}^m g_\sigma \operatorname{Tr} M_\sigma^T X - \operatorname{Tr} Q^T X \\ &= \sum_{\sigma=1}^m g_\sigma H_\sigma - \operatorname{Tr} Q^T X. \end{aligned} \tag{A5}$$

The strong duality theorem states that if the dual problem is *strictly feasible*, i.e., $\exists g : \sum_{\sigma=1}^m g_\sigma M_\sigma - Q \succ 0$ and $d^* > -\infty$, then $p^* = d^*$ and, in particular, p^* and d^* attain their supremum and infimum, respectively. In fact, the relaxed ground state problems that we describe in this article are strictly feasible, as one can always construct a mixed quantum state (corresponding to a particular vector g) that yields positive expectation values for all positive semidefinite constraint operators under consideration. Hence, there is no gap between the limiting points of the SDP and the solution is the actual infimum of the energy minimization problem.

During the optimization procedure, the program searches for data underlying an improved result for d^* or p^* within, or at the boundary of, convex cones. One cone is the set $\{X | X \succeq 0\}$ the other is $\{Z | Z = \sum_{\sigma=1}^m g_\sigma M_\sigma \succeq Q\}$. Different from, e.g., the simplex algorithm known from linear programming, which iterates along the boundary of the set of solutions, we make use of interior-point solvers, which show a superior performance in the context of SDP. These solvers consider modifications of the original optimization problem and advance along a path *within* the convex cone. Given certain assumptions, using interior point methods, the SDP can be solved to any desired numerical precision within polynomial time.

Appendix B: Anderson bounds

Anderson bounds [33, 34] are determined by splitting the Hamiltonian $\hat{H}$ into M terms $\hat{H}_m$ for which the ground state energies are accessible, for example, by choosing the terms $\hat{H}_m$ such that their supports are small enough to allow for an exact diagonalization of each term.

$$\hat{H} = \textstyle\sum_{m=1}^M \hat{H}_m \tag{B1}$$

The computation cost for determining the ground state energies of the operators $\hat{H}_m$ scales exponentially in the size of their spatial supports. One can exploit the sparseness of the Hamiltonians and access, with state of the art

computer resources, subsystem sizes of up to about 25 spins-1/2. Larger subsystems are difficult to address, as the $\hat{H}_m$ are not translation-invariant. With diagonal representations $\hat{H}_m = \sum_{m,n} E_m^n |m,n\rangle\langle m,n|$ and the lowest energy eigenstates $|m,0\rangle$, one has

$$\hat{H}_m \succeq \sum_{m,n} E_m^0 |m,n\rangle\langle m,n| = E_m^0 \cdot \mathbb{1} \quad \text{(B2)}$$

$$\Rightarrow \hat{H} \succeq \sum_m E_m^0 \cdot \mathbb{1}, \quad \text{(B3)}$$

i.e., $\sum_m E_m^0$ is a lower bound to the ground state energy of the Hamiltonian $\hat{H}$.

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